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Final report for the year 2001 on experimental and theoretical investigations of irradiation effects on physical and mechanical properties of iron and RAFM steels

Singh, Bachu Narain

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Final Report for the Year 2001 on Experimental and Theoretical Investigations of Irradiation Effects on Physical and Mechanical Properties of Iron and RAFM Steels

B.N. Singh

Risø National Laboratory, Roskilde
August 2003

Abstract

Effects of neutron irradiation on defect accumulation and physical and mechanical properties have been studied both experimentally and theoretically. Specimens of pure iron and RAFM (reduced activation ferritic-martensic) steels were irradiated to different dose levels and at different irradiation temperatures. The resulting microstructure was characterized using transmission electron microscopy, positron annihilation spectroscopy and electrical resistivity measurements. Mechanical properties were determined by uniaxial tensile testing. Dislocation-loop interaction, formation of rafts of loops, radiation hardening and formation of "cleared channels" were studied using different computational techniques.

Experiments have shown that nano-voids are formed both in pure iron and F82H steel already at 50°C. In pure iron, the formation of nano-voids is detected already at a dose level of $\sim10^{-3}$ dpa. Also in iron, self-interstitial atoms were found to accumulate in the form of glissile and sessile loops; at higher dose levels, these loops led to formation of rafts of loops. Irradiation led to an increase in the yield strength, a sudden drop in the yield stress, and, at higher doses, the initiation of plastic instability immediately beyond the upper yield point. Experimental as well as the results of computer simulations are found to be consistent with the cascade induced source hardening model.

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1 Introduction

Effects of neutron irradiation on damage accumulation and its impact on physical and mechanical properties of the reduced activation ferritic-martensitic (RAFM) steels are being extensively studied internationally since these alloys are considered to be candidate materials for the blanket and first wall of fusion reactors (e.g. DEMO and Commercial) [1]. These alloys are considered to have a number of more attractive properties than alternative structural materials like austeritic steels or vanadium alloys [2]. These considerations have led to the establishment of a comprehensive R&D programme within the framework of the European Fusion Technology Programme.

Although the ferritic–martensitic class of steels are very resistant to void swelling and maintains good fracture toughness at irradiation temperatures above 673K [3], they are prone to loss of ductility at lower irradiation temperatures [4, 5]. This is a matter of concern from the point of view of mechanical performance and lifetime of these alloys under fusion irradiation conditions, particularly when the mechanism controlling the loss of ductility is not understood. As regards the question of formation and growth of voids at relatively low temperatures (i.e. below the recovery stage V) and under the condition of a high helium generation rate in a fusion reactor, very little is known about its impact both on physical and mechanical properties. The present work was initiated to investigate systematically various aspects of damage accumulation including void nucleation and growth – as well as radiation hardening and radiation-induced loss of ductility both experimentally and theoretically. It was recognised, however, that the complexity of the intrinsic microstructure of these alloys does not render them suitable candidates for mechanistic studies. It was therefore decided to focus the theoretical investigations first on pure iron. In the following the main results of both theoretical and experimental investigations carried out during the year 2001 are summarised. Details of specific investigations are given in various articles and reports [6-10].

2 Materials and Experimental Procedure

Thin sheets (0.25 mm thick) of pure iron (99.9999%, C<0.01 ppm) were used to fabricate tensile specimens with 3 mm gauge width and 7 mm gauge length. These tensile specimens were irradiated in DR-3 reactor at Risø National Laboratory. Tensile specimens of another pure iron (of 99.995% purity) with a gauge length of 8 mm and gauge width and thickness of 1.5 and 0.25 mm were irradiated in the High Flux Isotope reactor (HFIR) at Oak Ridge National Laboratory. Both type of iron specimens were irradiated in fully recrystallised condition and had a grain size of about 30 μm. In the DR-3 reactor, the specimens were irradiated with a fast neutron flux of $2.5x10^{17}$ n/m^2s (E>1MeV) corresponding to a displacement dose rate of ~ $3.75x10^{-8}$ dpa (NRT)/s; dpa stands for displacement per atom. Irradiations were carried out at temperatures in the range of 50-350°C to a fluence of $1.5x10^{24}$ n/m^2 (E>1MeV) corresponding to 0.23 dpa (NRT). In the case of irradiations in the HFIR reactor at Oak Ridge, the neutron flux was about $4x10^{18}$ n/m^2s (E>1MeV) corresponding to a dose rate of about $6x10^{-7}$ dpa/s. Specimens were irradiated at ~ 70°C to fluences in the range from 4.5x

10^{20} to $4.7x10^{24}$ n/m^2 (E>1MeV) equivalent to displacement damage in the range from 10^{-4} – 0.8 dpa.

Both irradiated and unirradiated specimens were tensile tested at the irradiation temperature at a strain rate of $1.3x10^{-3}s^{-1}$ and in a vacuum of < 10^{-2} Pa.

For transmission electron microscopy (TEM) investigations, 1 mm wide ~ 0.1 mm thick strips were prepared from the irradiated materials and were electropolished at 20V in a solution of 20% perchloric acid in methanol at the ambient temperature. Thin foil were examined in a 200 keV JEOL 2000FX electron microscope.

The F28H and EUROFER 97 reduced activation steels were obtained from the common European stock available at PSI (Switzerland) in the as-tempered condition. Specimens from these steels were irradiated in as-tempered condition in the DR-3 reactor and BR-2 reactor at Mol (Belgium).

For each positron annihilation spectroscopy (PAS) measurement, two samples of approximately 5x3.5 mm^2 were cut from one tensile specimen. The samples were cleaned by electropolishing. A conventional positron lifetime spectrometer was used for PAS measurements.

The electrical conductivity measurements were made on the tensile specimens and were carried out as described in [11].

3 Modelling of Radiation Hardening and Plastic Instability

It was proposed already in 1997 that the irradiation-induced increase in the upper yield stress, the yield drop and plastic instability can be rationalised in terms of cascade induced source hardening (CISH) model [12]. The model is based on the assumption that the grown-in dislocations get decorated by glissile interstitial clusters produced in the cascades during neutron irradiation. Later, it was shown by analytical calculations using the linear elasticity theory that such dislocation decoration can occur [13]. However, it is not clear as to whether or not dislocation-loop and loop-loop interactions, particularly at close distances, can be calculated with enough accuracy within the framework of elasticity theory. It was therefore decided to carry out atomic scale simulations using molecular dynamics (MD) to eliminate this uncertainty [7].

For further validation of the idea that the grown-in dislocations do indeed get decorated by SIA clusters (loops) produced directly in the cascades, the techniques of dislocation dynamics and Monte Carlo have been utilised to study dislocation decorations [14] and the increase in the upper yield stress within the framework of CISH model [15].

The problem of plastic instability is considered to arise as a result of localisation of plastic flow immediately after the initiation of plastic deformation at and beyond the upper yield stress. As demonstrated by experiments, the flow localisation takes place in the form of "cleared channels" [16]. Fresh dislocations generated at dislocation sources glide very fast in the clear channels, interact with obstacles such as SIA loops and nano-voids present on the glide plane. Because of the repeated interaction of this kind, the obstacles from the glide planes of the cleared channels are removed. Computer simulations have been carried out using dislocation dynamics to study different stages of the "cleared channel" formation in neutron irradiated iron [14].

4 Results

4.1 Microstructural evolution

4.1.1 Transmission electron microscopy (TEM)

In order to evaluate the evolution of defect microstructure, the specimens of pure iron irradiated to doses between 10^{-4} and 0.72 dpa were investigated using transmission electron microscopy (TEM) and positron annihilation spectroscopy (PAS). The primary results from the TEM observation were as follows: There were no visible defect clusters observed in the lowest dose (10^{-4} dpa) iron specimen. The defect cluster size and density increased with increasing dose between 10^{-3} and 0.72 dpa. These observations suggest that defect cluster formation in fission neutron irradiated iron occurs via point defect nucleation and growth, as opposed to in-cascade formation of visible (>1 nm) defect clusters. It is interesting to note that in the specimen irradiated to 0.72 dpa, the interstitial loops were no longer present in the form of homogeneously distributed SIA loops. Instead, the CIA clusters were observed in the segregated form of rafts of SIA clusters. An example of raft of SIA loops in pure iron formed at a dose level of 072 dpa is shown in Fig. 1(a). Fig. 1(b) shows the dislocation loop microstructure of pure iron irradiated at 50°C in the DR-3 reactor to a dose level of ~0.4 dpa. Even though the loop distribution is reasonably homogeneous, in places there appears to be a tendency of loop agglomeration. This suggests that the formation of rafts of loops may start already at about 0.4 dpa. It is significant that in pure single crystal molybdenum the formation of raft begins to occur already at a dose level of ~10^{-2} dpa [17].

4.1.2 Positron annihilation spectroscopy (PAS)

The most direct way of illustrating the effect of irradiation on damage accumulation measured by PAS is the form of the positron lifetime spectra. Figs. 2 and 3 show such spectra measured for Fe and F82H, respectively, irradiated to a dose level of 0.23 dpa at different temperatures. It can be clearly seen that the accumulation of the irradiation-induced defects have significant effects on the positron lifetime. From Figs. 2 and 3 it is also evident that the lifetime spectra for Fe and F82H are qualitatively similar but quantitatively different, suggesting that the defect accumulation in these materials is noticeably different.

Quantitative analyses showed that the lifetime spectra for both Fe and F82H could be resolved into three lifetime components for all irradiation temperatures. The three lifetimes and the intensities of the two most long-lived components as functions of irradiation temperature are shown for both pure Fe and F82H steel in Fig. 4.

The annealing behaviour of iron specimens that were irradiated at 50 and 100°C is shown in Fig. 5. The lifetimes and intensities as functions of annealing temperature are shown by filled symbols (in red).

The positron lifetime spectra measured for pure iron irradiated at ~70°C to different doses are shown in Fig. 6. Clearly, the long-lived parts of the spectra become more intense with increasing irradiation dose level, showing at least qualitatively that the density and/or size of three-dimensional cavities increase with increasing dose.

In the quantitative analysis, the lifetime spectra could be resolved into three lifetime components for doses higher that 10^{-4} dpa. The result of the analysis is shown in Fig. 7. The two long lifetimes, τ_2 and τ_3 and the associated intensities, I_2 and I_3 arise from positrons that are trapped in three-dimensional vacancy clusters (i.e. nano-voids). As can be seen in Fig. 7, the general trend of the lifetime variation is that both τ_2 and τ_3 increase with increasing dose level from a value of about 230 ps, equivalent to a vacancy cluster of just 2-3 vacancies up to about 325 and 525 ps equivalent to 10 vacancies and more than 50 vacancies, respectively. Fig. 7 shows that both sizes and densities of three- dimensional vacancy clusters (nano-voids) increase with increasing dose level. Further analysis was carried out to determine the quantitative nature of the dose dependence of the nano-void density and the resulting void swelling and the results are shown in Fig. 8 (see [10] for details).

4.1.3 Electrical resistivity measurements

The electrical resistivity particularly of pure metals is sensitive to the concentration of lattice defects or their clusters in the lattice since they act as scattering centres for electrons. The technique of electrical resistivity measurement is therefore an effective technique to characterise the evolution of defect microstructure during irradiation or the decay of the defect microstructure during post-irradiation annealing. Furthermore, the technique compliments the information obtained by TEM and PAS. We have reported earlier, for example, the results on changes in electrical conductivity as a function of post-irradiation annealing temperature for pure iron irradiated at 100°C to a dose level of 0.23 dpa [18]. It was found that the recovery of the irradiation-induced defects took place in the same temperature range as observed by PAS. In addition, the electrical resistivity results clearly suggested that the transmutation produced impurities were affecting the electrical conductivity of iron.

Figure 9 shows the results of the electrical conductivity measurements for pure iron irradiated with fission neutrons at 50, 70 and 100°C; these measurements were made on the same specimens that were later used for the TEM and PAS investigations (see sections 4.1.1 and 4.1.2). As expected, the conductivity decreased with increasing dose level and decreasing irradiation temperature since the cluster density increases with increasing dose level and decreasing irradiation temperature. This is consistent with results of both TEM and PAS investigations. The low temperature data for specimens irradiated in HFIR and in DR-3 reactors are in good agreement, while the conductivities for the 100°C samples are clearly higher. This difference may be partly associated with trapping of defects by impurity carbon atoms below the migration temperature for carbon (> 70°C).

4.2 Mechanical Properties and Post-Deformation Microstructure

The engineering stress-strain curves for the unirradiated pure iron and the same iron irradiated at 70°C to different dose levels are shown in Fig. 10. It can be clearly seen that the yield strength increases and the uniform elongation decreases with increasing dose level. Furthermore, the ability of iron to work harden decreases with increasing dose level. It should be noted that the specimen irradiated to 0.72 dpa exhibits a strong yield drop, looses its ability to work harden and beyond the upper yield point deforms in an unstable fashion.

The specimens irradiated to ~ 0.4 dpa (in DR-3 reactor at ~50°C) and 0.72 dpa (in HFIR reactor at 70°C to 0,.72 dpa) and deformed at 50 and 70°C, respectively, were examined in TEM. The deformed microstructure was found to be dominated by the presence of “cleared channels”. In other words, the deformation of the irradiated materials occurs in a very localised fashion such that dislocations are generated only locally and these newly generated dislocations glide in the slip planes and interacts with loops and nano-voids in the slip planes. As a result of these interactions the loops and nano-voids are destroyed in the channels. Hence, the formation of the cleared channels. Fig. 11 shows examples of cleared channels formed in iron irradiated at 50 and 70°C, to dose levels of 0.4 and 0.72 dpa, respectively.

4.3 Modelling and Calculations

4.3.1 Cluster-dislocation interaction

Molecular statics was used to study the cluster-dislocation interaction energy at zero Kelvin in bcc iron lattice. The crystallites of about a million atoms were oriented along [100], [112] and [111] directions. The size along the Burgers vector, b, was approximately 15 nm along the dislocation line. The usual boundary conditions for static dislocation studies were applied, i.e. periodic along the dislocation line direction and rigid along the other two directions. An isolated dislocation was first introduced and relaxed. A cluster with the same Burgers vector as that of the edge dislocation was then created at a certain distance $r_{<110>}$ (e.g. along [110] direction) below the dislocation slip plane, e.g. below the extra half-plane and then the crystallite was relaxed again. The dislocation-cluster interaction energy was calculated using the energies of a previously-relaxed, isolated dislocation and a SIA cluster. The interatomic interactions were described by many-body potentials for α-Fe.

The interaction energy, E_{INT}, thus obtained was compared with the results of calculations using the full isotropic elasticity and the simple infinitesimal loop approximation. The results are compared in Fig. 12. It can be seen that the full isotropic elasticity calculations give satisfactory results for the interaction energy at distances larger than several dislocation core radii but overestimate the interaction force at short distances. The approximation of an infinitesimal loop gives satisfactory agreement on the interaction energy at large distances. These results suggest that in order to obtain the accurate interaction energy at distances shorter than a nanometer ($r_{<110>} \leq$ 1 nm), the influence of the real structure of the dislocation and the loop need to be taken into account. An important implication of the present results is that the interaction energy can be reliably estimated with the simple elasticity approach at separation distances much greater than it is possible to simulate using molecular statics.

4.3.2 Radiation Hardening and plastic instability

As mentioned already in section 3, recently the cascade induced source hardening (CISH) model has been proposed to rationalise the increase in the upper yield stress and a sudden yield drop in irradiated materials [12]. The model is based on the premise that during irradiation under cascade damage conditions, the grown-in dislocations get decorated with an atmosphere of small interstitial clusters and that this atmosphere prevents the grown-in dislocations from acting as dislocation sources. Later, it was shown analytically that such decoration is likely to occur by 1-D diffusing interstitial clusters produced in the cascades.

In order to verify the main conclusions of the analytical calculations and to gain further insight into the processes involved, a combination of Kinetic Monte

Carlo and 3-D Dislocation Dynamics computational techniques have been employed to study the phenomenon of dislocation decoration in bcc iron [14]. To study how glissile interstitial clusters migrate and interact amongst themselves and with the internal stress fields of the grown-in dislocations, a computational box of 400a x 400a x 400a ('a' is the lattice constant of bcc iron) is used with periodic boundary conditions. In order to study dislocation-cluster interaction and the decoration process, a dislocation loop lying on the <011> plane with Burgers vector ½ <111> is introduced into the simulation box. A number of interstitial clusters (of density varying in the range of $5 \times 10^{22} – 2 \times 20^{23}$ m^{-3}= are introduced in the box with random distribution and their initial jump directions are also randomly specified. The interstitial clusters are then allowed to diffuse one-dimensionally and interact amongst themselves and the grown-in dislocation loop (Fig. 13). When a cluster approaches the dislocation at distances closer than the "stand-off" distance (taken as 1.5 nm), the cluster is stopped. As can be seen in Fig. 13, the grown-in dislocation loop get decorated by the interstitial clusters in a very short time (6 ns).

The combination of the 3-D Dislocation Dynamic and Kinetic Monte Carlo computational procedures has been used also to determine the magnitude of hardening due to irradiation in bcc iron within the framework of the CISH model [15]. In the case of bcc iron, the main obstacles to dislocation motion are taken to be the nano-size voids. The density of these obstacles to glide plane is calculated from the experimentally measured values of the volumetric density of nano-size voids in pure iron neutron irradiated at 50 and 100°C to different dose levels. According to the CISH model a large number of dislocation sources are activated at the upper yield stress. These newly generated dislocations move on the glide planes and encounter the obstacles randomly distributed on the glide planes. Each dislocation segment is re3presented by a circular arc, and its curvature is determined by the applied stress, sum of all interaction forces and Burgers vector. When a dislocation segment encounters the nearest obstacle it splits into two segments and each segment continues to move until it reaches its equilibrium curvature or when the angle between the two tangents at the obstacle reaches a critical value, Φ_c. A KCM procedure is implemented to determine the probability of destruction of nano voids. This is calculated from the height of the energy barrier, the work done by the local forces at tangent points and the lattice temperature. After the annihilation of that nano voids, these two segments merge into one and the unified segment is advanced till it meets the next obstacle on the glide plane. Using this procedure, the stress level at the lower yield stress is obtained. The main results of these calculations are summarised in Fig. 14 for pure bcc iron neutron irradiated at 50 and 100°C to different dose levels. For comparison experimental results are also plotted in Fig. 14. The agreement between the calculated and the experimental results are reasonably good. The calculated results are somewhat lower probably because the effect of interstitial clusters is not included in the calculations.

As mentioned already in section 3, within the framework of the CISH model the problem of plastic instability is considered to be related to the phenomenon of plastic flow localisation in the form of "cleaned channels". In irradiated materials where grown-in dislocations get decorated with interstitial clusters such that they can no longer act as dislocation sources. At a certain level of the applied stress a large number of dislocations are released from sources giving rise to a sudden yield drop and in some cases plastic instability. Experiments show that under these conditions, dislocations activities are limited only to within the cleaned channels. Practically no dislocations are generated in the volume between the channels. This means that in order to understand the phenomena of plastic flow localisation, it is very important as to how the channels are initiated and how dislocations gliding interact with the obstacles in the glide planes and how these obstacles are finally destroyed making the cleaned channels very weak.

In the following some preliminary results of computer simulations experiments are described. These simulations also utilise the combination of Dislocation Dynamics and Kinetic Monte Carlo computational procedure. In the present work the main obstacles to dislocation motion in the glide planes are taken to be nano-voids, as found in experiments (see section 4.1) Under the action of an applied stress, dislocations generated from sources impinge on nano-voids and may destroy them if the work done by local forces exerted by dislocations on the nano-voids exceeds a critical value determined by the elastic interaction energy. In the present simulations, we assume that the nano-voids are destroyed by the gliding dislocations, once the angle between the arms of the dislocation that surround the void exceeds a critical value, Φ_c. Thus Φ_c is the only adjustable parameter in the present simulation.

Figure 15 shows the results of computer simulations for the stages of dislocation channel evolution in irradiated Fe [14]. Initially, dislocations in a local area of stress concentration or statistically low SIA cluster atmosphere density are activated when the local shear stress reaches a critical value. In Fig. 15(a), one such F-R source is activated at a stress level of 30 MPa. When the applied stress is increased to 65 MPa (Fig. 15(b)), several F-R sources are shown to have their dislocations bowing out in response to the applied stress and mutual interaction forces. However, only a few have expanded significantly to reach the edge of the simulation cube. Also shown in the same figure is the pre-annihilation stage of one of the F-R source dislocations, where two segments are about to annihilate, thus creating a full loop and restoring the initial pinned dislocation segment of the source. In Fig. 15(c), further activation of dormant F-R sources if achieved, when the local microvoid density is effectively reduced by the passage of nearby dislocations. A *domino* effect is this created, where the destruction of microvoids in a local region by one source activates other nearby sources. It is to be noted that the dislocation loop structure is not planar, because of the continuous climb process associated with each dislocation glide event. At a stress level of 70 MPa, dislocation loops start to impinge on the simulation box boundary, and at that point, periodic boundary conditions are implemented to inject those loop segments that emerge from one side of the boundary to the other side, as can be seen in Fig. 15(d) and (e). The evolution process is terminated when the leading-edger loop reaches the grain boundary or surface (which is assumed here to be 10 μm), and successive dislocation loops interact with one another to form a non-planar pileup of loops that would exert sufficient back stress on all sources to shut them off. The structure of the evolving non-planar pile-up of loops is shown from the side view in Fig. 15(f).

5 Summary

The main theme of the present report is to provide a brief description of activities dealing with various aspects of damage accumulation and its impact on physical and mechanical properties of pure iron and RAFM steels irradiated with fission neutrons at different temperatures. The evolution of defect microstructure has been characterised in detail using TEM, PAS and resistivity measurements. The corresponding effects of defect accumulation on mechanical properties has been characterised by uniaxial tensile testing. Post-deformation microstructure of irradiated materials has been investigated using TEM.

Experiments have demonstrated that nano-voids are formed both in iron and F82H steel already at the irradiation temperature of 50°C. In pure iron nano-voids have been detected at a dose level of as low as 10^{-3} dpa. Both irradiation and post-irradiation annealing experiments have shown coarsening of nano-voids at temperatures below the recovery stage V, indicating that migration and coarsening (via Brownian-like motion) of nano-voids may play a significant role in void nucleation. It is of interest to note that void swelling rate decreases rather rapidly with irradiation dose and reaches a very low value already at ~ 0.72 dpa.

The accumulation of the self-interstitial atoms occurs in the form of small clusters/loops the density of which increases with increasing dose level. These clusters begin to form rafts of loops at about 0.4 dpa and at 0.72 dpa the loop microstructure us completely dominated by the rafts of loops. As usual, the yield strength increases and ductility decreases with irradiation dose level. At a dose level of 0.72 dpa, the specimen shows a strong yield drop and beyond the yield drop deforms in a plastically unstable fashion. It is interesting to note that this mechanical response is observed at the dose level where the loop microstructure is dominated by the rafts of loops. Post-deformation microstructure showed that the plastic deformation occurs mainly in the "Cleared channels" and no significant amount of dislocation activities were observed in the volume between the channels.

Computer simulation studies were focussed on dislocation-loop interaction, formation of rafts of loops, the resulting hardening and finally the formation of cleared channels.

The dislocation-loop interaction was studied using MD technique and the results were compared with the results of elasticity calculations. It was found that the interaction energies can be accurately obtained using elasticity calculation for larger distances between a dislocation and a loop. However, for close-distance interactions, the effects of the structure of the dislocation and the loop may be important and should be determined using MD simulations.

The formation of rafts of loops has been studied using a combination of Dislocation Dynamics and Kinetic Monte Carlo computational techniques. Because of very high 1-D mobility of SIA clusters, the formation of rafts of loops occurs very rapidly. The simulation also shows that when SIA clusters are within a distance of several nanometers from each other and have their Burger vectors in parallel directions, will trap one another and trends to move in a self-organised group or raft. These results confirm the results of analytical calculations published already in 1977, [12, 13].

Using the same combination of simulation techniques, the increase in the upper yield strength as a function of irradiation dose has been calculated within the framework of CISH model [12]. The calculated results are found to be in good accord with the experimental results for iron irradiated at 50 and 100°C. Finally, the formation of cleaned channels (which are responsible for plastic instability) has been successfully simulated. In the calculations of both hardening and channel formation nano-voids are taken to be the main obstacles to dislocation motion on the glide planes.

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